

# Atomic Scale Ordering in Pt Nanoparticles

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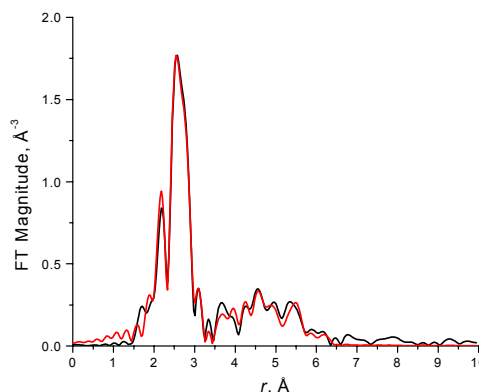
Abstract No. Fren8747

Beamline(s): X16C

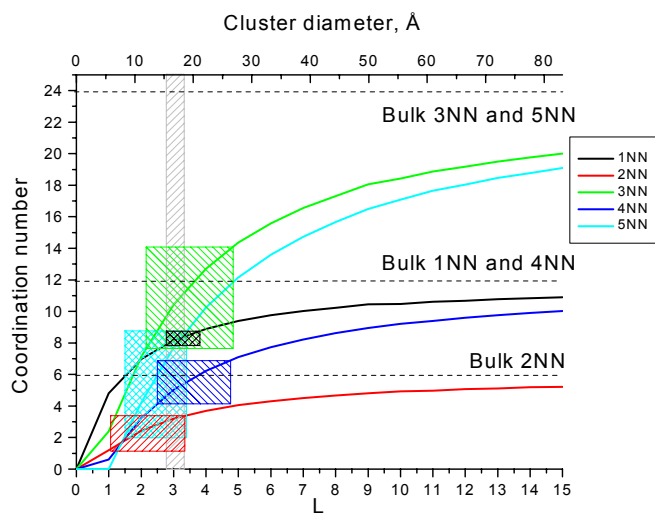
**Introduction:** EXAFS technique has unique yet not fully realized potential in solving the structure of nanoparticles. If the atomic environment beyond the first nearest neighbors to the absorbing atom is analyzed, the nanoparticle size, shape and surface orientation can be reliably determined.

**Methods and Materials:** We performed Pt  $L_3$  EXAFS analysis of fully reduced, metallic, carbon-supported Pt nanoparticles of three different sizes,  $\sim 20$  (sample S1), 40 (S2) and 80 Å (S3) in diameter. EXAFS was measured on X16C beamline, in transmission, at four different temperatures: 200 K, 300 K, 473 K and 673 K. The data were analyzed using FEFF7 theory [1] and UWXAFS data analysis package [2].

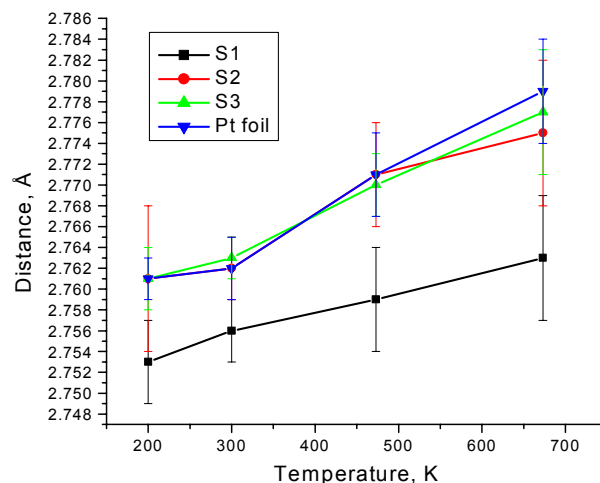
**Results and Conclusions:** From the five-shell fit (Fig. 1), we obtained the distribution of the coordination numbers in the five shells for all the nanoparticle sizes (Fig. 2). We measured 1NN bond lengths for all samples and at all temperatures (Fig. 3). The results were compared against different structural models with different size, shape and surface orientation of the nanoclusters. The results were in good agreement with the model of a hemispherical cuboctahedron with a 111-truncation by the plane of support,  $\sim 17$  Å in diameter, with Pt atoms occupying fcc sites, in excellent agreement with our STEM and electron microdiffraction results.



**Figure 1.** Fourier transformed EXAFS data (black) and fit (red) for the sample S1 with the  $\sim 20$  Å particles



**Figure 2.** Theoretical (lines) and experimental (boxes) coordination numbers, with their uncertainties, obtained for the S1 sample. The vertical dashed rectangle indicates the overlapping nanoparticle sizes as obtained from all coordination numbers for this model (111-truncated hemispherical cuboctahedron)



**Figure 3.** First nearest neighbor (1NN) distances as obtained from EXAFS analysis at different particle sizes and different temperatures. Apparent is the shortening of the mean 1NN bond length in the sample with the smallest particle size, due to the surface reconstruction caused by surface tension.

**References:** [1] S. I. Zabinsky, J. J. Rehr, A. Ankudinov, R. C. Albers, and M. J. Eller, "Multiple-Scattering Calculations of X-Ray-Absorption Spectra," *Phys. Rev. B* **52**, 2995, 1995.

[2] E. A. Stern, M. Newville, B. Ravel, Y. Yacoby, and D. Haskel, "The UWXAFS Data Analysis Package: Philosophy and Details," *Physica B*, **208 & 209**, 117, 1995.